N,N-Dimethyltrifluoroacetamide

Other names: Acetamide, 2,2,2-trifluoro-N,N-dimethyl-
CF3CON(CH3)2
Inchi: InChI=1S/C4H6F3NO/c1-8(2)3(9)4(5,6)7/h1-2H3
InchiKey: WXBWKMLIVXELSF-UHFFFAOYSA-N
Formula: C4H6F3NO
SMILES: CN(C)C(=O)C(F)(F)F
Mol. weight [g/mol]: 141.09
CAS: 1547-87-1

Physical Properties

Property code	Value	Unit	Source
affp	849.00	kJ/mol	NIST Webbook
basg	818.00	kJ/mol	NIST Webbook
gf	-616.93	kJ/mol	Joback Method
hf	-768.02	kJ/mol	Joback Method
hfus	12.56	kJ/mol	Joback Method
hvap	29.54	kJ/mol	Joback Method
log10ws	-0.50		Crippen Method
logp	0.637		Crippen Method
mcvol	84.080	ml/mol	McGowan Method
pc	3642.13	kPa	Joback Method
tb	351.81	K	Joback Method
tc	511.62	K	Joback Method
tf	221.43	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.93	J/mol×K	351.81	Joback Method
cpg	167.74	J/mol×K	378.45	Joback Method
cpg	176.08	J/mol×K	405.08	Joback Method
cpg	183.96	J/mol×K	431.72	Joback Method
cpg	191.40	J/mol×K	458.35	Joback Method

cpg	198.42	J/mol×K	484.99	Joback Method
cpg	205.03	J/mol×K	511.62	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1547871&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume